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FINAL TECHNICAL REPORT

AASERT: Triplet States of Small Molecules: Photochemistry, Spectroscopy, and Dynamics

Air Force office of Scientific Research
Grant Number F49620-97-0384

Co-Principal Investigators:

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Robert J. Silbey

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Period Covered: 01 June 1997 - 31 December 2000

I. Students Supported by AASERT Grant

A. Graduate Students

1. Selen Altunata (7/97-8/99, 12/99-2/00: 29 months)
2. Michelle Silva (7/97-8/99, 12/00: 27 months)
3. Leah Ruslen (1/99 - 3/99: 3 months)

B. Undergraduate Students

1. Susan Lang (Summer, 1997)
2. Mike Bonnet (Summer, 1997)
3. Simon Tisminezky (Spring, 1998)

C. Progress toward degree

AASERT funds were primarily used to support three female graduate students (Altunata, Silva, and Ruslen) and all three are currently in the final year of their Ph.D. programs. Their coursework and research has been of uniformly high quality.

The three undergraduates (Lang, Bonnet, Tisminezky) have all graduated from MIT with Bachelor's degrees. The AASERT-supported project played a particularly important role in establishing Susan Lang's scientific self-confidence and in defining her objectives for graduate study in Oceanography.

D. Specific Research Projects

1. **Selen Altunata's** research has been in the main area of our regular AFOSR grant. She has designed and assembled a second-generation, two-chamber, supersonic jet molecular beam apparatus for the study of triplet state structure and dynamics. Her new apparatus is now producing results vastly superior to those obtained in our original single chamber apparatus. In fact, by reducing the pressure in the detector chamber by a factor of ~ 100 , she has achieved one of the major goals of our triplet project: the SEELEM (Surface Electron Ejection by Laser Excited Metastables) spectra recorded on Cs and Au surfaces are profoundly different in shape and relative intensity (The Cs spectrum is $500\times$ more intense than the Au spectrum). This means that we now have independent probes of the S_1 and T_1 characters in each eigenstate.

Ms. Altunata has also developed statistical pattern recognition methods for extracting information about the mechanism of InterSystem Crossing (ISC). One paper has been published (JCP **113**, 6640-6651 (2000)) and a second one was recently submitted to the Journal of Chemical Physics.

2. **Michelle Silva's** primary research has been in the area of Intramolecular Vibrational Redistribution and Isomerization in singlet (both S_1 and S_0) acetylene (supported by a DOE grant). She has spent nearly a year at JILA in the laboratory of Dr. John Hall and Dr. Jun Ye attempting to record IR-IR double resonance NICEOHMS (Noise Immune Cavity Enhanced Optical Heterodyne Molecular Spectroscopy) spectra of $H^{13}C^{13}CH$. Her contribution to our AFOSR supported research is expertise in intracavity spectroscopy, servo systems for locking one longitudinal TEM_{00} mode of an optical cavity to the frequency of a scanned laser, and sum/difference frequency generation. Our studies of the spectra of molecular triplet states depend on the generation of <100 MHz spectral width tunable UV radiation by frequency quadrupling and pulse-amplifying a cw Ti:Sapphire laser.

3. **Leah Ruslen's** primary areas of research have been in Cavity Ring-Down Spectroscopy (CRDS) and combustion-related free radical kinetics. Her contribution to our AFOSR project is UV CRD spectroscopy of acetylene.

II. Publications

The following papers resulted from research partially supported by the AASERT grant.

1. S.J. Humphrey, C.G. Morgan, A.M. Wodtke, K.L. Cunningham, S. Drucker, and R.W. Field, "Laser Excited Metastable States of Acetylene in the 5.5 - 5.7eV Region," J. Chem. Phys. 107, 49--53 (1997).
2. H.K. Srivastava, A. Conjusteau, H. Mabuchi, A. Callegari, K.K. Lehmann, G. Scoles, M. L. Silva, and R.W. Field, "Ro-vibrational Spectroscopy of the $v = 6$ Manifold in $^{12}C_2H_2$ and $^{13}C_2H_2$," J. Chem. Phys. 113, 7376-7383 (2000)
3. S. Altunata and R. W. Field, "A Statistical Approach to the Study of the Singlet-Triplet Interactions in the 5.5 - 5.7 eV Region of Acetylene," J. Chem. Phys. 113, 6640-6651 (2000).
4. M. Silva, R. Jongma, R.W. Field, and A.M. Wodtke, "The Dynamics of Stretched Molecules': Experimental Studies of Highly Vibrationally Excited Molecules with Stimulated Emission Pumping," Ann. Rev. Phys. Chem.
5. S. Altunata and R. W. Field, "An Assumption-Violating Application of the Lawrance-Knight Deconvolution Procedure: A Retrieval of Electronic Coupling Mechanisms Underlying Complex Spectra," J. Chem. Phys.

III. Interactions/Transitions

1. Talks by R. Field, K. Cunningham, and S. Altunata at the 52nd (1997), 53rd (1998), 54th (1999), and 55th (2000) "International Symposium on Molecular Spectroscopy (Ohio State University)"

Talk by Selen Altunata at Wesleyan University (2000)

Talks by Robert Field at national ACS meetings (Spring, 2000 and Pacificchem 2000), Edwards Air Force Base (Spring, 2000), International Conference on Photochemistry (San Juan, Puerto Rico, April, 2000), Kobe University (May, 2000), Argonne National Lab (October, 2000), University of California, Riverside (December, 2000).

2. Collaborations with scientists (S. J. Lipson and J. A. Dodd) at Hanscom Air Force Base, which resulted in three publications:

M.P. Jacobson, S.L. Coy, R.W. Field, S.J. Lipson, R.B. Lockwood, D.L. Vitito, W.A.M. Blumberg, and P.S. Armstrong, "Numerical Pattern Recognition Analysis of CO Atmospheric Simulation Experiments," J. Phys. Chem. 104, 249-257 (2000).

A.F. Ruckstuhl, M.P. Jacobson, R.W. Field, and J.A. Dodd, "Baseline Subtraction Using Robust Local Regression Estimation," J. Quant. Spectr. Radiat. Transf. 68, 179-193 (2001).

E. S. Hwang, J. B. Lipson, R.W. Field, and J. A. Dodd, "Detection of OH (X,v) via the $B^2 + - X^2$ Transition and Properties of the $B^2 +$ State," J. Phys. Chem.

IV. New Discoveries, inventions, patents: None.

V. Honors

Robert Field: Doctor of Science (honoris causa), Amherst College, May, 1997.

Robert Field: Elected to Fellowship in the American Academy of Arts and Sciences, 1998.

Robert Field: Haslam and Dewey Professorship, 1999.

Susan Lang: Dreyfus Undergraduate Research Fellowship, 1997.

Susan Lang: Chemistry Department Prize for Undergraduate Research, 1999.